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Thermodynamics of magnetic systems from first principles MARKUS EISENBACH, Oak Ridge National Laboratory, GREGORY BROWN, Florida State University, AURELIAN RUSANU, University of Tennessee, DON M. NICHOLSON, Oak Ridge National Laboratory — Density functional calculations have proven to be a useful tool in the study of ground state properties of many materials. The investigation of finite temperature magnetism on the other hand has to rely usually on the usage of empirical models that allow the large number of evaluations of the system's Hamiltonian that are required to obtain the phase space sampling needed to obtain the free energy, specific heat, magnetization, susceptibility, and other quantities as function of temperature. We have demonstrated a solution to this problem that harnesses the computational power of today's large massively parallel computers by combining a classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) for constrained magnetic states. Here we will present recent advances in our method that improve the convergence as well as applications to 3d element based ferromagnets. This research was performed at Oak Ridge National Lab and sponsored in parts by the Center for Nanophase Material Sciences, Scientific User Facilities Division, the Center for Defect Physics, an Energy Frontier Research Center funded by the US DOE Office of Basic Energy Sciences and the Division of Materials Science and Engineering, Office of Basic Energy Science of

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